THERMOELECTRICITY IN METAL ORGANIC THIOLATE COORDINATION POLYMERS

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : Institut Lumière et Matière and IRCELYON

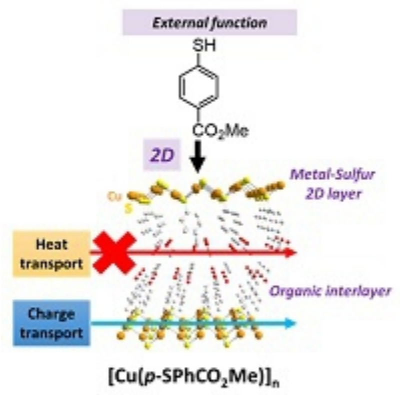
LEVEL : M2
TEAM(S) : LUMINESCENCE
MMCI
ENERGIE

CONTACT(S) : PAILHES Stéphane

CONTACT(S) DETAILS: stephane.pailhes[at]univ-lyon1.fr / Tel. 0472431018

KEYWORD(S) : thermoelectricity / Coordination Polymers

SCIENTIFIC CONTEXT :



2D-Thermoelectric Metal Organic Thiolates Coordination Polymers

Thermoelectricity allows the conversion of heat losses into electricity (Seebeck effect) or conversely to cool down and regulate a temperature under the effect of an electric current (Peltier effect). Aside from our reliance on fossil fuel, one of the challenges of the energy use is the huge untapped amount of waste heat generated. To tap this mostly unused resource, efficient thermoelectric materials need to be developed to convert waste heat into renewable electricity. Coordination polymers (CPs) are a new class of metal-organic crystalline frameworks that has the potential to revolutionize a wide range of technologically and industrially relevant fields especially in solid-state sensing and energy conversion devices. The very rich chemistry of CPs allows to design the metallic channels (their doping level and dimensionality), the complexity and porosity of the surrounding organic matrix as well as the coupling between the organic and inorganic frameworks. The basic concept is to bury metallic channels within a complex organic matrix which is very efficient to diffusive the heat as sketch in the Figure. Our objectives are to evaluate the potentiality of these materials for the thermoelectric conversion and optical applications and secondly, to understand the limiting factors for guiding the design of new structures.

MISSIONS :

We offer a M2 internship (6 months) with the possibility of thesis funding focused on the experimental and theoretical (ab initio) studies of the electrical and thermal transport as well as optical properties, and related thermoelectric effects in conducting thiolate-based CPs. Recently, we have discovered a new promising structure and composition of thiolate-based CPs (paper under submission). Its thermoelectric properties have been experimentally and theoretically determined. According to our ab initio simulations, the goal of the internship will be to investigate the change of its properties (structural and physical) with doping in order to change the position of the electrochemical potential in the electronic band structure and compare with the simulations. The experimental study involves the macroscopic electronic and transport measurements in a wide temperature range and the investigations of the electronic structure by photoemission. The results will be first interpreted on the basis of our ab inito simulations.

OUTLOOKS :

Experimental and theoritical studies of the thermoelectric properties in this new conducting CPs

published on 02/11/2022